International Journal of Engineering Research (ISSN : 2319-6890)
Volume No.2 Issue No7, pp : 432-437 01 Oct. 2013

Soil-Water Characteristic Curve Modeling at Low Water Content: Empirical and Semi-Empirical Approaches

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ABSTRACT :
In this paper, we evaluate the performance of the most widely used semi-empirical models (van Genuchten (1980), Fayer and Simmons (1995) and Fredlund and Xing (1994)) and, an empirical model, the Modified Kovacs (MK) model for the determination of soil-water characteristic curve at the low water contents of two horizons of a soil from Burkina Faso. Combining terms from capillary state and adsorbed state of soil water gives a physical basis for the Modified Kovacs model. Our study confirms that the use of semi-empirical models requires somewhat large dataset covering the entire range of water content while the empirical model MK requires only basic geotechnical properties of soil and a few experimental points to adjust the parameters m and a_c of the model. It appears that the MK model, by its simplicity and lower cost for the acquisition of experimental data, is the most appropriate.

Keywords : soil, water, arid, modelling, empirical, semi-empirical

1. INTRODUCTION

The water content in the unsaturated soil is a function of soil water chemical potential. This constitutive relationship is commonly referred to as the soil-water retention curve in soil sciences, and well known as the soil-water characteristic curve (SWCC) in geotechnical engineering. Soil-water characteristic curve appears to be a key hydrodynamic parameter in the fields of soil science and civil engineering. Using the SWCC, one can compute or determines the hydraulic conductivity function [1], the volumetric variation of the soil [2], the shear strength in the unsaturated soil [3], and the attribution of the water content in subsurface [4].
While knowledge of the two extreme states of water in a soil (saturated and very dry conditions) seems well advanced, the unsaturated state at medium to low water content deserves further investigation. This condition is usually encountered in soil surface layers where strong interactions occur between soil and roots, microorganisms or building foundations. In arid and semi-arid zones, **best** knowledge of physical flow processes at low water contents would allow development of more effective tools for water resources management.
Despite the relatively small amounts of water retained, accurate representation of soil water characteristic curves at the dry end is important for modeling biological processes including plant water uptake and microbial activity in arid environments [5]. Accurate measurement over the full range of water contents is a delicate task. Most or all methods for measuring the water potential have limitations, especially at intermediate and low values of the water content (pendular and hygroscopic states). **Frequently** the curve is completed by extrapolation, which can lead to instabilities in numerical codes [6]. Experimental methods (infiltration and/or drainage, evaporation and condensation) associated with inverse problems also suffer from shortcomings, including in the instrumental devices, and are mostly robust only at the higher water contents (i.e., the funicular state) where the liquid phase is continuous. **It arises from this** the question of the validity at low water contents of the **matrix** head - water content relationship, h - θ, usually a key function to describe the physics of unsaturated flow. Indeed, this range of the water content comprises the pendular state where the liquid and vapor phases presumably are discontinuous, and the hygroscopic state where only the gas phase is continuous, while water is being strongly adsorbed onto the solid phase. This is **the reason** why **one** prefers the use of the water chemical potential to describe the movement of water in all of its states. One of the fundamental properties of the chemical potential stipulates that at local thermodynamic equilibrium, the potential of a component present in two phases should be the same [7]. Experimentally well-defined methods (e.g., [7]) should apply to all important parts of the soil water characteristic curve, from saturation to oven dryness.
The main objective of this study is to evaluate the models representating the SWCC in the range of low water contents for an arid soil of Burkina Faso. These results will be used in the modeling of water transfer and management of water resources in arid areas. A comparison is made between the two modeling approaches in low water contents given the constraints of time and cost. This with a view to retain a relatively simple and less expensive method for arid soil hydrodynamic properties determination.

2. MATERIAL AND METHODOLOGY

2.1. TYPICAL SOILS FROM BURKINA-FASO

Morphological Characteristics
Two kind of natural soil from Nasso (Burkina-Faso) are under investigation. The first kind, denoted NH1, was taken from the top layer of ground (0-30 cm depth) and the second one, denoted NH2 comes from deeper layer (30-70 cm depth). Morphological properties are summarized in Tab. 1. Physical analyses have been realized by dry sieving after washing (standard NF P94-056) for particles larger than 80

µm and sedimentation analysis (standard NF P94-057) for smaller particles. Soils granulometric curves are ploted in Figure 1. According to ISSS classification, the textural typologies of these soils are sand for NH1 and loamy sand for NH2 what corresponds globally to sandy soils. Bulk density, ρ_s, of each sample have been measured using the Core Sampler Method on undisturbed soil (standard NF X31-501). Assuming the soil particle density to be ρ_d = 2650 kgm^{-3} leads to determine the saturated mass water content w_{sat} :

$$w_{sat} = \rho_w \left(\frac{1}{\rho_s} - \frac{1}{\rho_d} \right) \quad (1)$$

where ρ_w is the density of water, taken as 1000 kg.m^{-3}.

Table 1 : Physical properties of soils used

	Particle size distribution %			**Bulk Density**
Soil type	Sand	Silt	Clay	kg.m^{-3}
NH1	90	7	3	1688
NH2	85	6.5	8.5	1652

Measurement of soil water retention curve

The soil water retention curve was determined by combining measures from tensiometry and sorption isotherms. Following the ideas put forth by [7], the water content is plotted as function of the water chemical potential, denoted µ in J.kg^{-1}, rather than pressure head or suction. Indeed, a variety of micro-scale mechanisms governs soil/water interactions and liquid pressure cannot be defined for low water content. From its energetic definition, the chemical potential can consistently describe the thermodynamic state of water over the whole range of water content. It can be seen as a unifying concept well defined from a thermodynamic framework. Classical experimental devices were used: (i) pressure plate apparatus at constant temperature (30°C) for high water contents corresponding to the funicular state; (ii) saturated saline solutions for low water contents in the hygroscopic state. For both methods, at equilibrium, mass water content was calculated by differential weighting after oven-drying at 105°C for 48 hours.

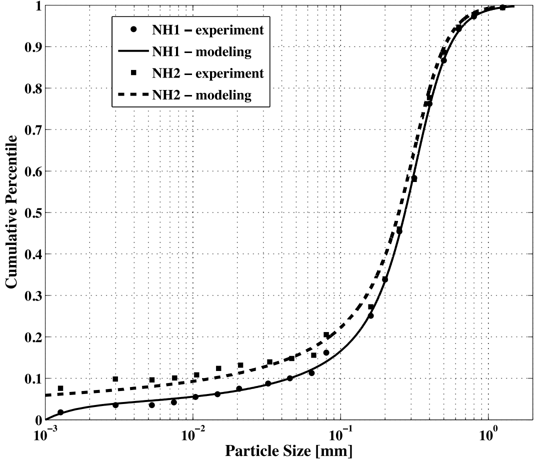


Figure 1 : Soil granulometric curves

2.2. THEORETICAL MODELLING

Semi-empirical approach

It consists to find an analytical expression that takes into account the variables that influence the flow of the water in the soil. The resulting models are currently based on the distribution of the pore size, distribution of particle size or relationships between measurable characteristics of soil. In formulations underwritten, µ is the absolute value of the water chemical potential.

(i) VG80 [1], where fitting parameters are: w_r, α, n and m:

$$w = w_r - \left(w_{sat} - w_r\right)\left[1+\left(\alpha\mu\right)^n\right]^{-m} \quad (2)$$

(ii) FS95 [10], with w_a, α, n and m as fitting parameters and μ_0= 10^6 Jkg^{-1} :

$$w = w_a\left(1 - \frac{\ln \mu}{\ln \mu_0}\right) + \left[w_{sat} - w_a\left(1 - \frac{\ln \mu}{\ln \mu_0}\right)\right]\left[1+\left(\alpha\mu\right)^n\right]^{-m} \quad (3)$$

(iii) FX94 [12], where fitting parameters are w_r, n, m, μ_r and μ_i:

$$w = \left[1 - \frac{ln\left(1+\frac{\mu}{\mu_r}\right)}{ln\left(1+\frac{\mu_0}{\mu_r}\right)}\right] \frac{w_{sat}}{\left[ln\left(e+\left(\frac{\mu}{\mu_i}\right)^n\right)\right]^m} \quad (4)$$

Numerical minimization procedure based on Levenberg-Marquardt algorithm was applied to objective function (Eq. 5), an ordinary weighted least-squares method, to identify optimal parameters values for each semi-empirical model.

$$O\left(\vec{b}\right) = \sum_{i=1}^{N} W_i\left[w_i - \hat{w}_i\left(\vec{b}\right)\right]^2 \quad (5)$$

where $\vec{b}$ is a vector whose components are all the unknown parameters of the model to identify, N is the number of data pairs for the retention function, W_i is the class weight of the individual water content and w_i, $\hat{w}_i$ are the measured and model predicted values, respectively.

Empirical approach

Several functions are available in the literature. We chose to evaluate an empirical method for determining the soil water curve from basic geotechnical properties proposed by [16]: modified Kovács (MK) model. This model has been successfully evaluated by the authors on the basis of several types of plastic and non-plastic soils, especially in consideration of the thermodynamic states of water in soil: capillary water and adsorbed water.

The MK model is represented by a series of equations that have been developed considering that water is retained in granular materials by capillary forces, which are responsible for capillary saturation (S_c), and adhesion forces causing saturation for adhesion (S_a) [16]. Thus, according to the MK model, the degree of saturation S_e in materials depends on two components, S_c and S_a. These components are originaly express in terme of matric head h (cm). One can show that the suction or matric potential ψ (in Pa) and the matric head h (in m), both widely used in soil hydrology, are closely

(ISSN : 2319-6890)
01 Oct. 2013

related to the chemical potential μ (J.kg^{-1}) [7]. The relationship between matric potential, chemical potential and matric head is given by $\mu=\psi/\rho_w=gh$, where ρ_w is the density of water and g the acceleration of gravity (m.s^{-2}).

$$S_e = \frac{\rho_s}{\rho_e n} w = 1 - \left(1 - S_c\right)\left\langle 1 - S_a \right\rangle \qquad (6)$$

$$S_c = 1 - \left[\left(\frac{h_{co}}{h}\right)^2 + 1\right]^m \exp\left[-m\left(\frac{h_{co}}{h}\right)^2\right] \qquad (7)$$

$$S_a = a_c \left\{1 - \frac{\ln\left(1+\frac{h}{h_r}\right)}{\ln\left(1+\frac{h_0}{h_r}\right)}\right\} \frac{\left(\frac{h_{co}}{h_n}\right)^{2/3}}{e^{1/3}\left(\frac{h}{h_n}\right)^{1/6}} \qquad (8)$$

In equation (6), $\langle . \rangle$ represents the Macauley brackets ($\langle x \rangle = 0.5\left(x + |x|\right)$) and w (kg.kg^{-1}), n (-) are the gravimetric water content and the porosity respectively. In equations (7-8), h_{co}(cm) is an equivalent capillary height, a reference parameter in MK model. It is related to an equivalent pore diameter, with depend to the solid surface area. For granular materials, h_{co} is obtained from the following relationship:

$$h_{co} = \frac{0,75}{eD_{10}\left[1 + 1,17\log\left(C_U\right)\right]} \qquad (9)$$

where D_{10} (cm) is the diameter corresponding to 10% passing on the cumulative grain-size distribution ; $C_U = D_{60}/D_{10}$, the uniformity coefficient and e, the void ratio.
The parameter m in equation (7) is a pore size coefficient that controls capillary saturation and can be related to C_U ($m = 1/C_U$). In equation (8), a_c is an adhesion coefficient ; h_n, a normalization parameter introduced for unit consistency ; h_0, the matric head which induces water content of zero ($h_0 = 10^7$ cm for thermodynamic considerations) and h_r (cm), the residual matric head. h_r can be estimed with h_{co} :

$$h_r = 0,86 h_{co}^{1,2} \qquad (10)$$

The MK model is easy to use. Just have the basic geotechnical properties namely bulk and soil particle densities to compute n and e; the particle size distribution to extract D_{10} and D_{60}.

3. RESULTATS AND DISCUSSION

3.1. SEMI-EMPIRICAL APPROACH

Saturated water content of each horizon of soil is evaluated through relation (1) with parameters values from Table 1. Tables 2-3-4 summarize the models evaluated for the water retention curve, the values of descriptive parameters identified for soils horizons NH1 and NH2. The values of statistical parameters determining the performance of the models in representing the experimental values as the coefficient of determination, R^2, and standard deviation, RMSE (Root Mean Square Error), are recorded in this table.

Table 2 : VG80 SWCC parameters values

	Model parameters					Statistics	
	w_{sat}	w_r	α	n	m	R^2	$RMSE$
	kg.kg^{-1}	kg.kg^{-1}	kg.J^{-1}	-	-	%	kg.kg^{-1}
NH1	0.215	0	0.912	1.392	0.282	99.3	0.0048
NH2	0.223	0	1.902	6.736	0.042	99.5	0.0052

Table 3 : FS95 SWCC parameters values

	Model parameters					Statistics	
	w_{sat}	w_a	α	n	m	R^2	$RMSE$
	kg.kg^{-1}	kg.kg^{-1}	kg.J^{-1}	-	-	%	kg.kg^{-1}
NH1	0.215	0.033	0.437	1.615	0.507	99.8	0.0038
NH2	0.223	0.046	1.544	3.536	0.127	99.7	0.0042

Table 4 : FX94 SWCC parameters values

	Model parameters					Statistics	
	w_{sat}	n	m	μ_r	μ_i	R^2	$RMSE$
	kg.kg^{-1}	-	-	J.kg^{-1}	J.kg^{-1}	%	kg.kg^{-1}
NH1	0.215	1.648	0.932	50.03	2.086	99.8	0.0033
NH2	0.223	2.023	0.604	59.41	1.067	99.9	0.0029

Figures (2) to (3) represent the experimental and modeled water retention curves for horizons NH1 and NH2. In general, good correlation is obtained between theoretical models and experimental values. The very low standard deviation (RMSE) and very close values of 100% for the coefficient determination R^2 (Tables 2-3-4) are illustrative.

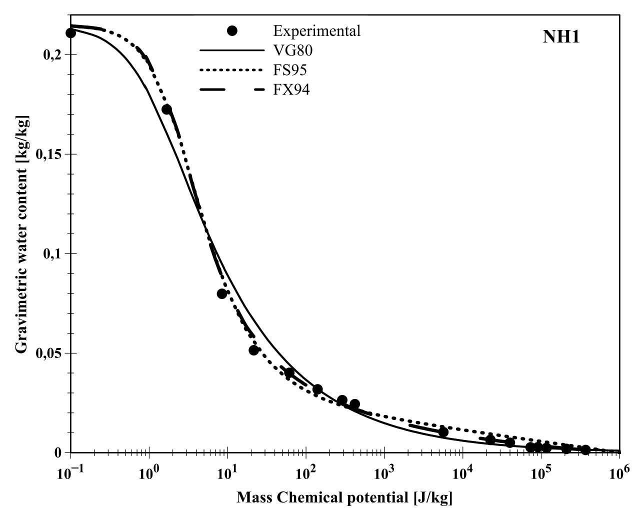


Figure 2 : Experimental and fitted theoretical SWCC: horizon NH1.

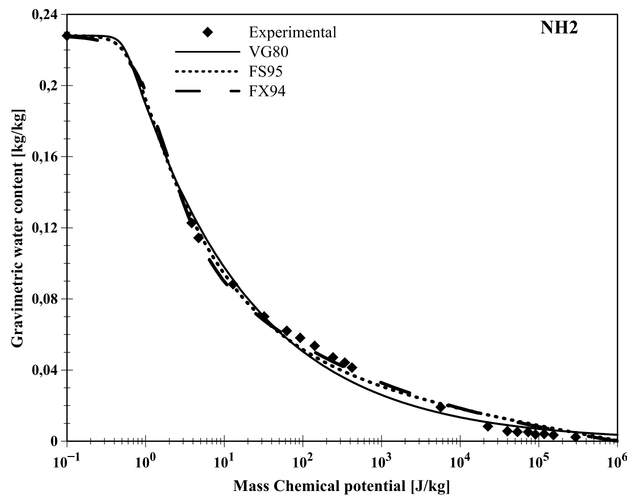


Figure 3 : Experimental and fitted theoretical SWCC: horizon NH2.

Based on these statistical values, the model FX94 is the most representative with R^2mean = 99.84%, followed by the model FS95 with R^2mean = 99.74% and finally the most popular model, VG80 where R^2mean = 99.41%. However, in low water contents, differences are remarkable for the various models tested (Fig. 4) and (Fig. 5). For the sandy material NH1, FX94 is the most efficient while for sandy loam material NH2, the results are mixed. VG80 model, sometimes, fails to reproduce experimental values at low water content [8,10]. Forcing moisture content value to zero for a chemical potential of 10^6 J.kg^{-1} in FX94 and FS95 could be the cause for a soil with more fine particles.

In addition, the extensions models from FX94 and FS95 in low water contents support the hypothesis by [9]: a linear variation in semi-log between the water content and the chemical potential in the lower margin of the water retention curve. This assumption has restriction for materials containing more fine particles (clay soils). Several studies show that water retention properties in the dry end of the soil are strongly correlated with the specific surface area which increases with the clay content of the soil [5,16]. A proportional relationship between water content and logarithm of the chemical potential is often used to represent the water retention curve in this oven-dry condition [13,17]. Thus, the main challenge is to find a mathematical model, doubly differentiable, to connect the two extreme soil conditions (high saturation and very dry end) where available models seem effective in reproduction of experimental values of the water retention curve.

Another serious concern with regard to models of water retention curves, is the ease of use in a numerical problem of water transfers. When the relation $\mu = f(w)$ is used, it is very difficult or impossible to obtain an analytical expression derived from the water retention curve models from FX94 and FS95 [8]. This constraint greatly restricts the use of these models in simulation codes of water transfers, which is not the case for VG80.

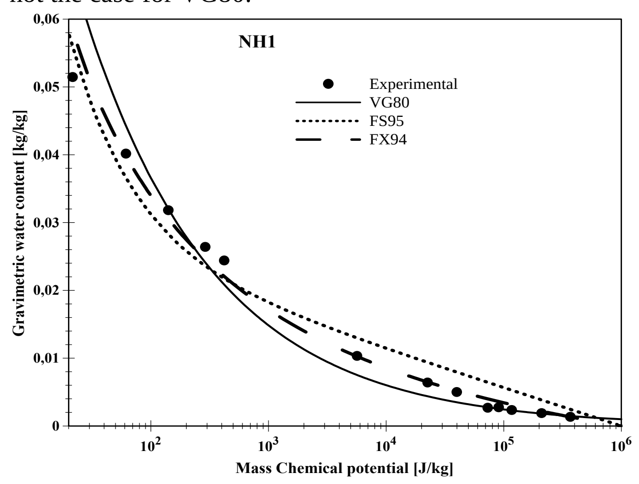


Figure 4 : Experimental and fitted theoretical SWCC: zoom at low water content for horizon NH1.

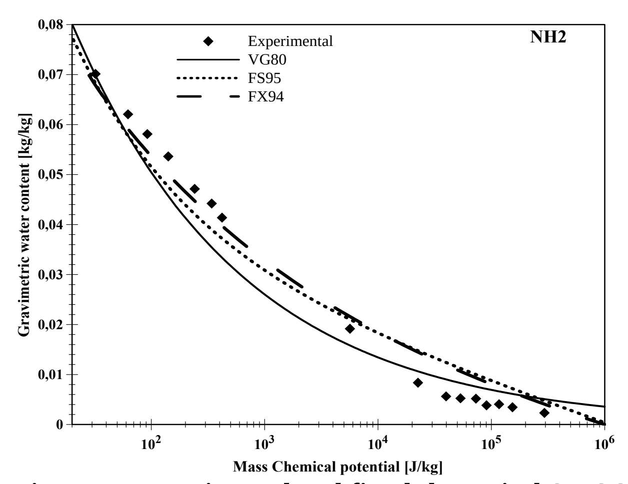


Figure 5 : Experimental and fitted theoretical SWCC: zoom at low water content for horizon NH2.

3.2. EMPIRICAL APPROACH

The Modified Kovàcs model was tested for the two non-plastic granular soil horizons NH1 and NH2. The values of basic geotechnical parameters (n, e, ρ_s, D_{10}, D_{60}), derived from the characterization of physical properties are used to calculate the characteristic curves from the set of equations (6) to (10).

The important parameters for the model are the coefficient of adhesion a_c acting in the of adsorption component S_a and m, the pore size coefficient in the capillary state. [16] suggested the values a_c = 0.01 and $m = 1/Cu$ for granular materials (no plastic, no cohesive). Using these values for the horizon NH1 gave mixed results shown in Figure (6).

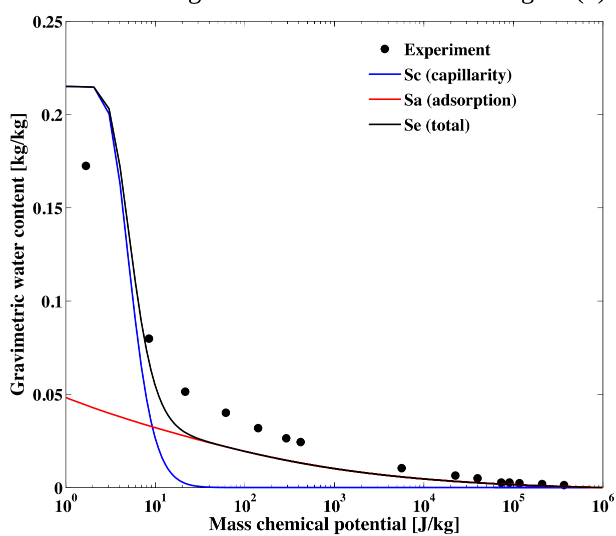


Figure 6 : Experimental and fitted theoretical SWCC for horizon NH1 with empirical values of *m* and a_c proposed by [16].

Using our experimental data, it is possible to adjust the parameters a_c and m for each material tested to better represent the experimental points in any part of the curve, this is shown in Figure (7) for NH1 and Figure (8) for NH2. Four (04) experimental data regularly distributed on the curve are sufficient to adjust these parameters. The adjusted values are: a_c = 0. 018, m = 0.031 for NH1 and a_c = 0.0115, m =0.002 for NH2.

The model describes well the curve at the low water contents. At high saturation state, results are less representative. However, this model is a good basis for characterization of the water retention curve from data which can be acquired in a limited time and cost. His performance in low water contents are a major asset in the characterization of hydrodynamic properties of sandy soils in arid and semi-arid regions for optimization and management of water resources.

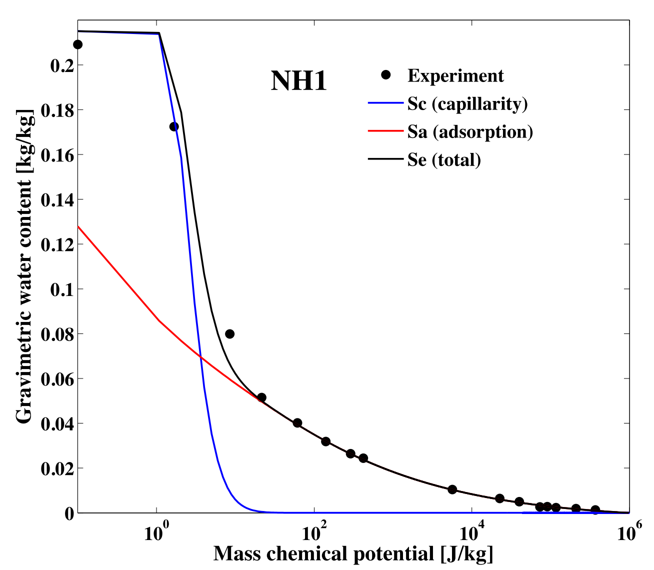


Figure 7 : Experimental and fitted theoretical SWCC for horizon NH1 with empirical values of *m* and a_c ajusted with experimental data.

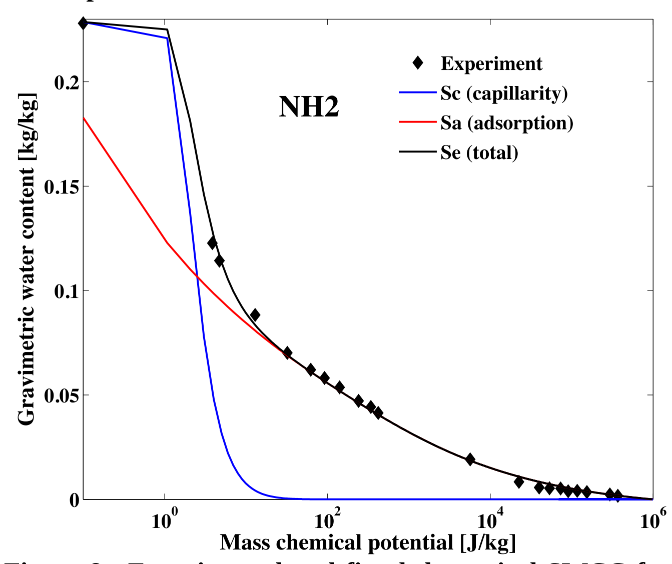


Figure 8 : Experimental and fitted theoretical SWCC for horizon NH2 with empirical values of *m* and a_c ajusted with experimental data.

4. CONCLUSION

Two modeling approaches are used to determine the soil-water characteristic curves of two soil horizons from Burkina Faso. They represent typically the major part of soils in arid and semi-arid regions, regularly subjected to water stress increased by rare rainfall and extreme temperatures. Thus, particular emphasis is focused on the low water contents part, intermediate state between high water saturations and oven-dry states.

It appears from the study that Modified Kovacs model, an empirical approach model, is more appropriate to estimate the curve at low water contents compared to the semi-empirical approach models evaluated. Combining terms from capillary state and adsorbed state of soil water gives a physical basis for the Modified Kovacs model. The use of semi-empirical models require enough data from the curve over the entire range of water content while the empirical model MK requires only basic geotechnical properties of soil and a few experimental points to adjust the parameters *m* and a_c of the model. It would be useful to refine correlation functions between these parameters and the physical properties of soil from a large database covering the entire range of soil textural. Additional investigation may also be oriented on estimation of unsaturated hydraulic conductivity, the other soil hydrodynamic function, from the basic geotechnical properties.

ACKNOWLEGDEMENT

The authors would like to acknowledge Fondation 2iE (Ouagadougou – Burkina Faso, www.2ie-edu.org) for physical characterisation of materials in his laboratory (Laboratoire Eco-Matériaux de Construction - LEMC). We especially wish to François TSOBNANG, Adamah MESSAN and Koffi KOKOLE.

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